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SHOCK TUBE MEASUREMENTS FOR LIQUID FUELS COMBUSTION

ARO Contract Number DAAD19-01-1-0597

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SUMMARY/OVERVIEW:

We report results of basic research aimed at improving knowledge of the combustion behavior of diesel and jet-related fuels. The work is intended to develop a reference database of gas-phase chemical kinetics and two-phase spray measurements applicable to engine modeling. Research is being conducted in three Stanford shock tube facilities and focuses on two topics: (1) shock-induced ignition time and species time-history measurements and comparisons with current detailed kinetic models of jet fuels and cyclo-alkanes at both high and low pressures; (2) fundamental studies of fuel spray evaporation rates and ignition times of low-vapor pressure fuels such as JP-8, diesel fuel and normal alkane surrogates in a new aerosol shock tube using state-of-the-art optical diagnostic and imaging techniques.

TECHNICAL DISCUSSION:

Validation of reaction mechanisms and development of new and improved reduced mechanisms describing the pyrolysis, oxidation and ignition of practical fuels require a reliable database of experimental combustion targets. Only a limited amount of shock tube ignition time data presently exist for the heavier practical fuels and fuel components, and these data exhibit substantial scatter and are of varying reliability. Stable species data from flames or bench-top reactors exist and have been used to partially validate reaction mechanisms, but little or no data is available on small transient radical species, such as OH, HCO, CH_3, and benzyl, that play important roles in ignition processes. To help remedy these deficiencies, we are currently building a new database of ignition time and species concentration time-history measurements derived from shock tube studies. This database will cover: fuel components such as n-alkanes, branched alkanes, cyclo-alkanes, alkenes and aromatics; surrogate mixtures; and practical fuels including gasoline, kerosene and diesel. Current work is described below.

Methylcyclohexane: Though we have measured ignition times in aromatic species, e.g. toluene, little data exists for cyclo-alkanes. Recently, we have measured ignition delay times of methylcyclohexane (MCH) over a range of conditions: 1.3 to 2.9 atm, 1225 to 1560 K, X_{MCH} from 0.25% to 1%, and equivalence ratios from 0.5 to 2. An initial correlation for the ignition time of MCH was generated, see Fig. 1. These preliminary results have been compared with the existing data and current model of Orme, Curran and Simmie (2006) and though there is agreement in magnitude, there is a significant difference in activation energy. High-pressure ignition experiments to continue testing of these mechanisms are planned. As MCH readily condenses in the mixing manifold and shock tube, a species-specific method to measure low *in situ* fuel concentration is needed for accurate ignition time measurement. Accordingly, we have

developed a mid-IR (3.39 μm) laser absorption detection scheme to accurately measure fuel concentration in the shock tube; the advantages of this direct fuel-loading sensor are applicable to other practical and surrogate fuels.
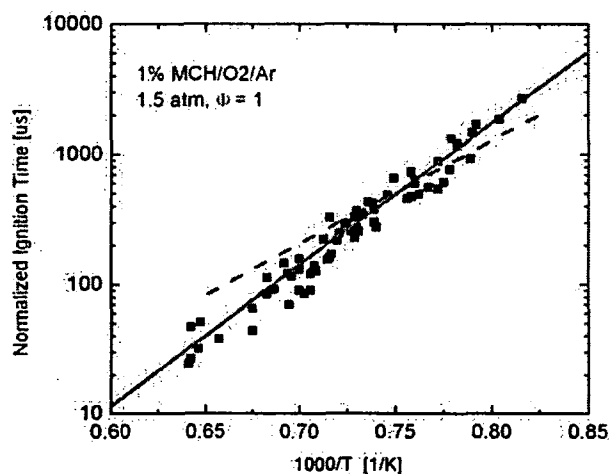

Fig. 1. Ignition delay times: 1% methylcyclohexane/O_2/Ar, $\Phi = 1$, 1.5 atm. Dashed line: Orme et al. 2006 mechanism. Solid line: best fit to current data, $\tau_{ign} = 7.5 \times 10^{-14}$ $P^{-0.96}$ $X_{MCH}^{-0.82}$ $\Phi^{1.47}$ exp(25560/T) [s].

Jet Fuel and Kerosene: We are continuing our experimental and modeling study of the ignition time of jet fuel. We have completed modification of our high-pressure shock tube facility (HPST) which will allow improved experimental control in the preparation of test gas mixtures of liquid fuels. We have compared the predictions of several current kinetic mechanisms for jet fuel and used these mechanisms to predict and plan our upcoming set of high-pressure (15 to 60 atm) ignition time experiments. [1]

n-Heptane and Iso-Octane: Methyl radical concentration time-histories were measured during the oxidation and pyrolysis of iso-octane and n-heptane behind reflected shock waves. [2] Initial reflected shock conditions covered temperatures of 1100 to 1560 K, pressures of 1.6-2.0 atm and initial fuel concentrations of 100-500 ppm. Methyl radicals were detected using cw UV laser absorption near 216 nm; three wavelengths were used to compensate for time- and wavelength-dependent interference absorption. Methyl time-histories were compared to the predictions of several current oxidation models. While some agreement was found between modeling and measurement in the early rise, peak and plateau values of methyl, and in the ignition time, none of the current mechanisms accurately recover all of these features. Sensitivity analysis of the ignition times for both iso-octane and n-heptane showed a strong dependence on the reaction $C_3H_5+H=C_3H_4+H_2$, and a recommended rate was found for this reaction. Sensitivity analysis of the initial rate of CH_3 production during pyrolysis indicated that for both iso-octane and n-heptane, reaction rates for the initial decomposition channels are well isolated, and overall values for these rates were obtained. The present concentration time-history data provides strong constraints on the reaction mechanism of both iso-octane and n-heptane oxidation, and in conjunction with OH concentration time-histories and ignition delay times, recently measured in our laboratory, should provide a self-consistent set of kinetic targets for the validation and refinement of iso-octane and n-heptane reaction mechanisms.

Fundamental Kinetics Database Utilizing Shock Tube Measurements: We have published Volume 1 of this database on-line at http://hanson.stanford.edu/. [3] This volume includes ignition delay time measurements and details of species concentration time-history profiles from shock tube experiments at Stanford University. Fuel species included in this database include: hydrogen, methane, and ethylene; normal alkanes including ethane, propane, n-butane, n-heptane and n-decane; branched alkanes including iso-butane, iso-pentane, and iso-octane; JP-10;

butadiene; toluene; gasoline and ternary gasoline surrogates. Fuels for which high-pressure ignition delay time data exist includes hydrogen, methane, n-heptane, iso-octane, toluene, gasoline, and gasoline surrogates. Also included in the database are OH concentration time-history measurements for most of these fuels, and CH, CH_3, and CO_2 measurements for the small fuels. Work is continuing on database development including: interaction with model developers, measurements of higher hydrocarbons including soot formation, and an extension of this database to a wider pressure range and lower temperatures relevant to flameless oxidation.
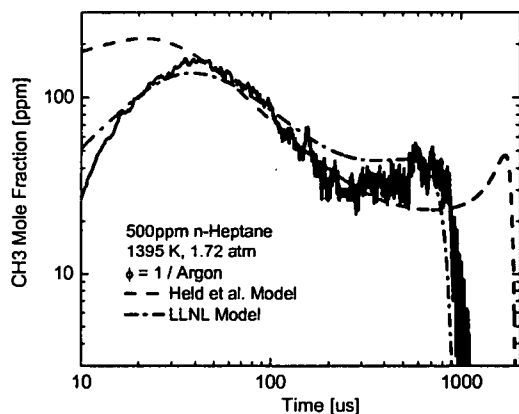

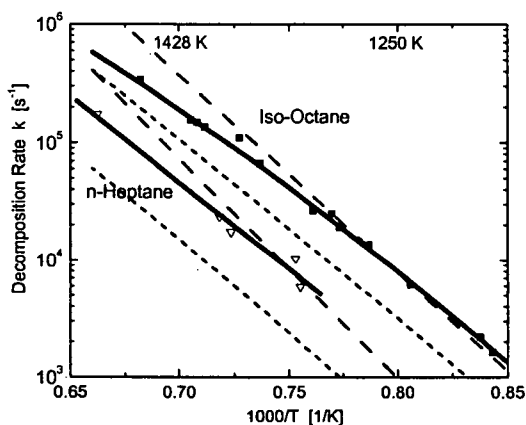Fig. 2. Example methyl absorption data: n-heptane oxidation.

Fig. 3. First-order decomposition rates k for iso-octane and n-heptane, 1.75 atm. Upper three lines, iso-octane; lower three lines, n-heptane. Solid lines, fit to data; dashed lines, Davis and Law rates; short dashes, Curran et al. LLNL rates.

Aerosol Shock Tube: Ignition Time Measurements of Low-Vapor-Pressure Fuels: We have developed a method to measure shock tube ignition delay times in low-vapor-pressure fuels without heating the shock tube. This method which uses the aerosol shock tube has several advantages, not the least of which is that we do not heat and chemically react the fuel in a heated shock tube before the ignition time experiment. It also permits the direct measurement of ignition times at high concentrations for fuels such as JP-8 and diesel and surrogates such as decane, dodecane and hexadecane. To quantify the amount of fuel in our mixtures for these experiments we have developed two fuel diagnostic methods: one using multi-wavelength Mie extinction for liquid fuel loading and one using gas phase absorption, both with IR lasers. Figure 4 presents initial n-dodecane/air ignition times for an equivalence ratio of 0.66 and 8 atm measured using the aerosol shock tube. This amount of fuel loading would require heating to over 50 C in a conventional shock tube. We have found no previous experimental work at these fuel loadings. Experiments are in progress to extend these measurements to decane, hexadecane, JP-8 and diesel fuel for a wider range of reaction temperatures and pressures, and to include investigations of soot formation.

Measurements of Droplet Evaporation behind Shock Waves: We have developed a suite of tools for studying aerosols behind shock waves. These include the aerosol shock tube itself, a laser-based Mie-extinction particle sizing diagnostic, a tunable near-infrared laser diagnostic for vapor concentration, and a one-dimensional computational model. With these tools, we measured the behavior of water aerosols in the range of 1-10 μm behind shock waves with temperatures between 450-600 K and pressures between 0.65-1.1 atm. See Fig. 6. From these data we

determined evaporation rates and found a correlation that provides the non-continuum evaporation rate in terms of a d^2 evaporation rate and a correction function. [4]
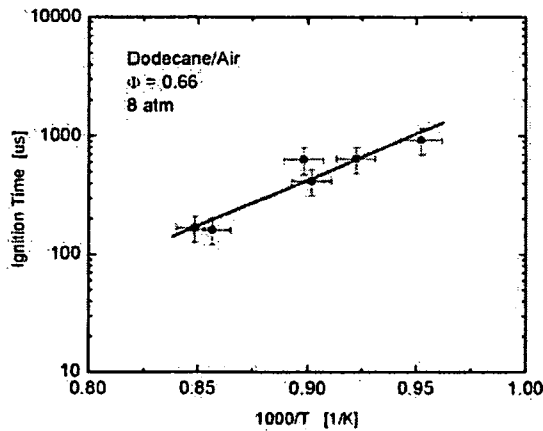

Fig. 4. Ignition delay times: n-dodecane/air, 8 atm, Φ = 0.66. Data derived using the aerosol shock tube.
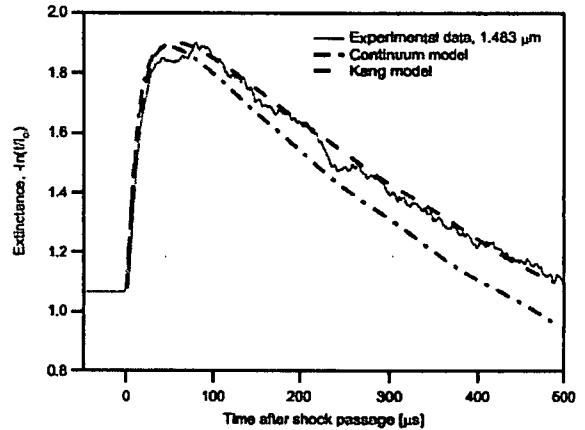
Fig. 5. Water droplet evaporation: experimental and model. Pre-shock conditions: 223 torr, 295 K; with a log-normal droplet distribution parameters: d = 2.8 μm, k = 1.48; and droplet loading of 9.9 ppmv. The incident shock speed is 513 m/s, and the immediate post-shock conditions are 0.85 atm and 458 K.

ARO-SPONSORED PUBLICATIONS (2005-2006):

1. S. Vasu, D. F. Davidson, R. K. Hanson, "Shock Tube Ignition Delay Times and Modeling of Jet Fuel Mixtures," submtted for publication, 42nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, 2006.

2. D. F. Davidson, M. A. Oehlschlaeger, R. K. Hanson, "Methyl Concentration Time Histories during iso-Octane and n-Heptane Oxidation," accepted for publication, Proceedings of the Combustion Institute 2006.

3. D. F. Davidson and R. K. Hanson, "Fundamental Kinetics Database Utilizing Shock Tube Measurements," Mechanical Engineering Department Report, Stanford University, November 2005.

4. T. C. Hanson, D. F. Davidson, R. K. Hanson, "Shock Induced Behavior in Micron-Sized Water Aerosols," submitted for publication, Physics of Fluids 2006.